Application No. 10,000,000
Applicant: Dan E. Rosenthal
Title: Method for Analytical Jacobian Computation in Molecular Modeling
Sheet 1 of 4



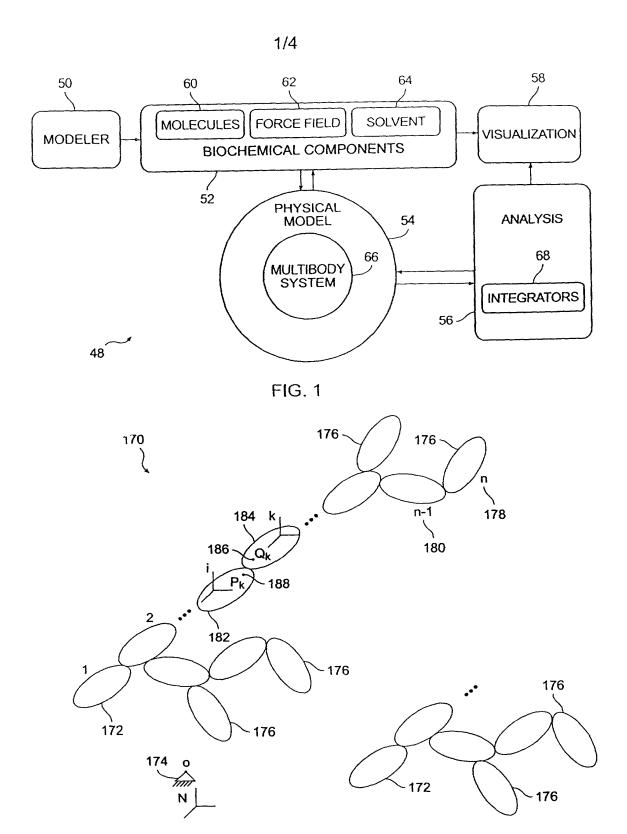


FIG. 2

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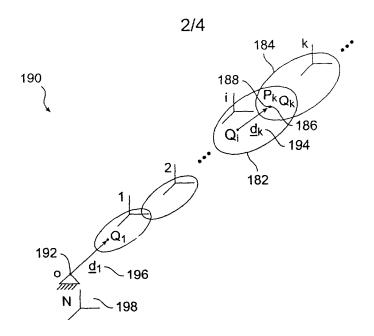


FIG. 3

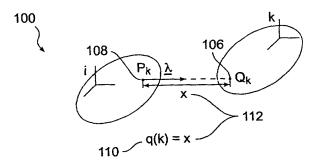


FIG. 4A

102
$$\begin{array}{c}
108 \\
\downarrow \\
P_{k} \\
\downarrow \\
06 \\
106 \\
110 \\
q(k) = \theta
\end{array}$$
114

FIG. 4B

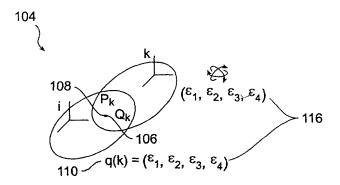


FIG. 4C

RESIDUAL FORM METHOD	DIRECT FORM METHOD
TO COMPUTE ρ _q AND ρ _u	TO COMPUTE q AND û
 COMPUTE THE FIRST KINEMATICS CALC. AND THE FIRST KINEMATIC RESIDUAL ρq(k) GENERATE Î(k), THE SPATIAL LOAD BALANCE FOR EACH BODY COMPUTE DYNAMIC RESIDUAL ρu(k) 	 COMPUTE ἀ USING JOINT SPECIFIC ROUTINES PERFORM FIRST KINEMATICS CALC. WITH ἀ = 0 GENERATE RESIDUALS ρ_u AND NEGATE ρ_u = -ρ_u PERFORM SECOND KINEMATICS CALC. COMPUTE ὰ USING FORWARD DYNAMICS

COMPARISON OF METHODS

FIG. 5

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4/4 ANALYTIC JACOBIAN METHOD

1. COMPUTE THE ANALYTIC JACOBIANS OF THE KINEMATICS ROUTINES:

$$J_{qq} = \frac{\partial (Wu)}{\partial q}$$
 AND $J_{qu} = W$

- 2. COMPUTE $z \triangleq -M^{-1}\rho_u(q, u, 0)$ USING THE DIRECT METHOD
- 3. COMPUTE THE ANALYTIC JACOBIANS OF THE DYNAMICS RESIDUAL ROUTINE

$$\frac{\partial}{\partial q} \, \rho_u(q,\, u,\, z) \;\; AND \quad \frac{\partial}{\partial u} \rho_u(q,\, u,\, z)$$

4. BACKSOLVE FOR THE ANALYTIC JACOBIAN OF THE DYNAMICS ROUTINE USING RESULTS FOR $\,z\,$ FROM THE SECOND KINEMATICS STEP:

$$J_{uq} = \frac{\partial \dot{u}}{\partial q} = -M^{-1} \frac{\partial \rho_u(q,\,u,\,z)}{\partial q} \quad \text{AND} \quad J_{uu} = \frac{\partial \dot{u}}{\partial u} = -M^{-1} \frac{\partial \rho_u(q,\,u,\,z)}{\partial q}$$

FIG. 6

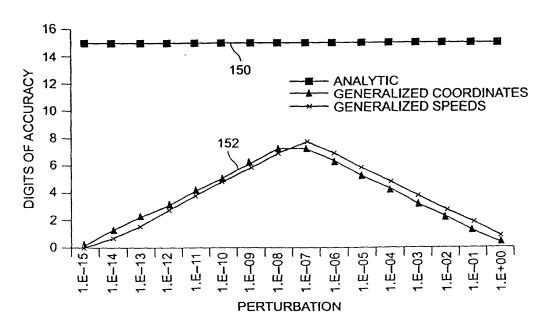


FIG. 7